

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.87            | 0.81 | 0.87           | 0.82 | 0.86       | 0.86 |

Model Results

Predicted value: 4.51e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.87e-01

Confidence level: 3.22e-01

Nearest Neighbors from the Training Set

|   |  |  |
|---|--|--|
| <div>Image not found</div> <div>Endosulfan</div> <div>Measured: 1.14e-06</div> <div>Predicted: 6.37e-06</div>         | <div>Image not found</div> <div>Endosulfan I</div> <div>Measured: 1.14e-06</div> <div>Predicted: 6.37e-06</div>  | <div>Image not found</div> <div>Endosulfan II</div> <div>Measured: 1.14e-06</div> <div>Predicted: 6.37e-06</div> |
| <div>Image not found</div> <div>Methabenzthiazuron</div> <div>Measured: 2.67e-04</div> <div>Predicted: 1.49e-03</div> | <div>Image not found</div> <div>Lenacil</div> <div>Measured: 2.56e-05</div> <div>Predicted: 1.78e-04</div>   | <div>Image not found</div> <div>Cinchonine</div> <div>Measured: 7.44e-04</div> <div>Predicted: 4.26e-04</div>    |
| <div>Image not found</div> <div>Cinchonine</div> <div>Measured: 7.44e-04</div> <div>Predicted: 4.26e-04</div>         | <div>Image not found</div> <div>Thioperoxydiphosphoric acid<br/>([(HO)2P(S)]2S2), tetramethyl<br/>ester</div> <div>Measured: 4.00e-05</div> <div>Predicted: 7.24e-05</div> |  |

